

CHALCOGEN-BONDED TETRAFLUORO-1,3-DITHIETANE WATER COMPLEX: WHAT DOES IT TAKE TO INVERT THE WATER?

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The rotational spectrum of the water adduct of tetrafluoro-1,3-dithietane has been investigated by using high resolution rotational spectroscopy. Experimental evidence and quantum theoretical analyses revealed that the two moieties are linked together through a dominant S-O chalcogen bond. The rotational transitions of four isotopologues are split into two component lines due to the internal rotation of the water moiety around its C_2 axis. In the HDO isotopologue, a small μ_c dipole moment component is generated which inverts upon water internal rotation, allowing the experimental determination of the tunneling splitting (21.46(5) GHz). Flexible model calculations can reproduce this splitting when the barrier to water internal rotation is 87.4(2) cm^{-1} .